COUPLING FINITE AND DISCRETE ELEMENT METHODS USING AN OPEN SOURCE AND A COMMERCIAL SOFTWARE

Ákos Orosz, Kornél Tamás, János P. Rádics, Péter T. Zwierczyk
Department of Machine and Product Design
Budapest University of Technology and Economics
Műegyetem rkp. 3., H-1111, Budapest, Hungary
E-mail: orosz.akos@gt3.bme.hu

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ABSTRACT

There are many cases where mechanical engineering structures interact with bulk materials, e.g. cultivating and mining machines.
The tool of the machine has effect on the aggregate and vice versa. The aggregate puts complex forces on the machines. These loads are usually simplified and replaced with a mean, distributed force, which is the input of further computations (e.g. finite element (FEM) simulations). This can be done, because the difference between two different, but statically equivalent loads becomes very small at sufficiently large distances from load. However, near the area, where loads act, the results using the simplification are not real, therefore finding the optimal tool design is difficult.
The discrete element method (DEM) models the materials using particles (elements) with independent translational and rotational degrees of freedom and arising forces (interactions) between them. This allows the simulation and tracking of each particle independently, which makes DEM ideal for modelling bulk materials. The FEM is usually used for modelling continua. If DEM is coupled with FEM, the result is a detailed stress distribution near the loads. In the possession of the detailed stress state, the optimization of the tool can be performed, and a better construction may be created.

INTRODUCTION

In the field of mechanical engineering, there are many types of machines which were designed to handle bulk materials. Good examples are the ones which came into interaction with stone aggregates: stones are yielded, crushed, transported and deposed by massive and complex machines to be finally used in e.g. railway ballasts and road base courses. The crushed rock aggregates are essential additives of concrete and asphalt mixtures. The tools of the machines are affected by static and dynamic loads from the interaction with stones, which cause high level of wear and the risk of fatigue.
Another important field, where machine tools interact with bulk materials is the agricultural machinery. The mechanical characteristics of the inhomogeneous soil are highly nonlinear. The tools of the different machines turn over, rip, compress and mix the soil to raise productivity. The efficiency of these processes is highly affected by the shape of the tools. The effect of the soil on the tool cannot be neglected, as it causes remarkable abrasion.
The various types of sands, similarly to stone aggregates, are needed to be yielded, transported and sorted which is also done by machinery. The solid pharmaceutical industrial products must be treated carefully, which requires the precise design of the geometry and material of the machine tools.
The examples show the wide variety of machinery, which came into interaction with bulk materials. The design and optimization of these structures are traditionally relying on the routine of practice or applying approximation equations. These methods require the manufacturing of several prototype variants and carrying out a large number of benchmark tests to find the best concept.
The numeric simulation of different processes creates the opportunity to virtually test the construction variants in the phase of conception creation, which reduces the number of manufactured prototypes, thus reducing the cost of design and validation process significantly.

SIMULATION METHODS

Discrete Element Method

The discrete element method (DEM) is a numerical technique where the material is made up from discrete elements (particles). The elements have independent motional and rotational degrees of freedom (DoF). The model can track the finite displacements and rotations (possibly deformations) of the particles. Interaction forces can be risen and extinguished between the elements (Bagi 2007, Cundall and Hart 1992).
Because of the definition, the behaviour of the model depends on two factors: the properties of the particles (shape and material) and on the characteristics of interactions (constitution law). The element type is chosen based on the features of the original material, as well as the constitution law, but parameters of interactions between elements have to be calibrated.

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The Finite Element Method

The finite element method (FEM) (Zienkiewicz 1971) is most often used to model continuum materials. Its major application fields are the simulation of mechanical (static, dynamic, buckling, fatigue), thermodynamic and electrodynamic processes.
The finite element method (FEM) also models the material with limited number of elements, however, the adjacent elements have common nodes. These nodes have common DoF (Dill 2012).
So, the similarity between FEM and DEM is that both describes the material with finite number of elements, however, these elements are not independent in case FEM, where the neighbouring elements have common nodes (with same DoF). This makes FEM more suitable for modelling continua and DEM for describing bulk materials.

THE MODELLING POSSIBILITIES OF MACHINE TOOLS

As the main goal of DEM simulations in the field of mechanical engineering is to model the interaction between the machine and the handled material, both the machine tool and the treated substance have to be modelled, which can be done in different ways. The DEM gives a good solution for modelling bulk materials, but there are multiple solutions for describing the tool of the machine depending on the needed information and computational efficiency. There are models that are based on purely the DEM (e.g. using zero thickness elements or cohesive interaction law), but the coupling of DEM and FEM is also a possible way.

The Use of Elements with Zero Thickness

There are two DEM element types, which are ideal for modelling boundary conditions and the geometry of tools.
The *wall* element is an infinite plane with zero thickness, which is usable to separate half-spaces. It has the same constitutional model as the volume elements have, so it is able to come into interaction with them, which arises e.g. repulsive and shear forces.
The *triangular facet* elements are defined by 3 points in 3D space. They have also zero thickness, and the capability to come into interaction with volume elements. In the right constellation, they can represent any surface, so they can be used to model machine tools with complex geometry. Such a geometry can be created by exporting parametric models in STL format using computer aided design software. Figure 1 shows a shaft represented by triangular facets.

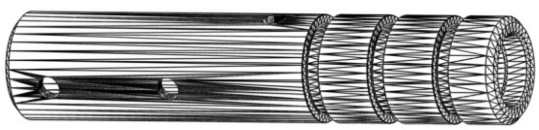

Figure 1: A shaft made up of triangular facet elements

Zero thickness elements model the tool as an ideally rigid body, so they can be used only if the deformations of the tool have so little influence that they can be neglected. Zero thickness elements give information about the load distribution affecting the tool.

The Use of Bonded Interactions

Besides the modelling of granular media, DEM is capable to simulate continua. It can be done by defining the interactions in the way that they have tensional resistance (cohesion). Figure 2 represents the uniaxial tension test of a material with cohesive constitutional model.

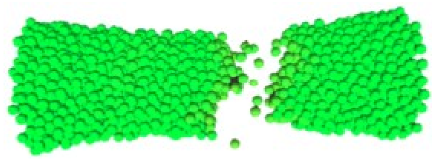

Figure 2: Tension test of a cohesive material made up of sphere elements (Šmilauer et al. 2015)

The advantage of modelling the tool with cohesive DEM elements is the potential to simulate deformations, cracks, breakage and wear. The stress field in the body is also computable by analysis of interaction forces. The disadvantage of such model is in the creation process, as finding the optimal constitutional model and calibrating its parameters takes considerable effort and time.

One-Way Coupling

To get the stress distribution and deformations of the tool, the FEM can be connected (coupled) with DEM. If the deformations of the tool are small, the so-called one-way coupling can be carried out. Where different data (e.g. force, velocity field) are computed via DEM are imported into the FEM simulation as a condition. It can be done with a special interface or a text file in the appropriate format. Such a series of simulations can be seen on Figure 3.

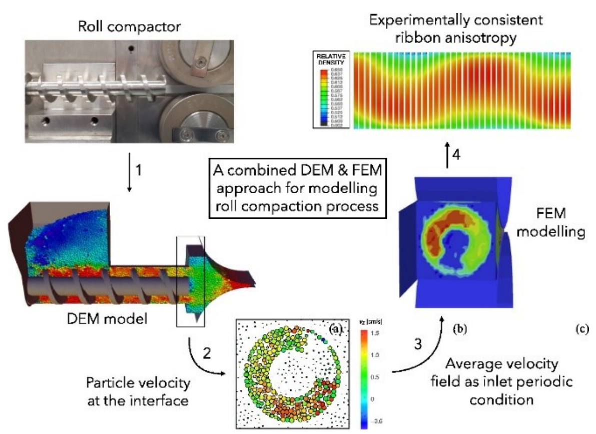

Figure 3: Flow Diagram of a Complex Roll Compactor Analysis (Mazor et al. 2017)

The DEM and FEM simulation are carried out in different software in most cases. The main task is to create the connection between the programmes and create the corresponding geometries. If the connection is established, the one-way DEM-FEM coupling provides an effective solution to find the stress distribution of a machine tool at small deformations with a low a computational demand.

Two Way (Parallel) Coupling

In reality, the interaction of the tool and the bulk material is dual. The moving tool shapes the bulk material, but this substance also deforms the tool. A deformed tool has slightly different effect on the material from the original one, which affects the forces on the tool etc. If the magnitude of this deformation is small, the one-way coupling can be used, else a new model is needed.
The solution is the creation of a two-way (parallel) simulation. In this case, the tool is made of a finite element mesh (Figure 4), which is able to establish contacts with discrete elements.

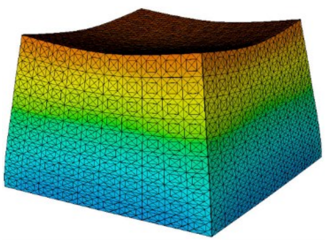

Figure 4: A geometry made of finite element mesh (Xiang et al. 2009)

The two-way coupling technique is also capable to create deformable elements by defining an internal finite element mesh. (Figure 5).

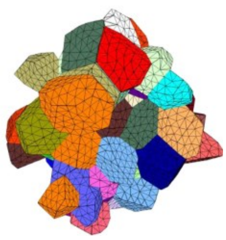

Figure 5: Polyhedron elements which contain internal finite element mesh for modelling crystalline solids (Li et al. 2017)

The method requires the interactive, real-time cooperation of a DEM and an FEM software, or a complex program, which have both DEM and FEM core. Due to the switching between the two models, iterations are needed where the conditions of the convergence are hard to define. For the same reason the simulations are computationally demanding, but in case of the proper definition, the solution will be accurate.

CREATING A ONE-WAY CONNECTION

The interaction of a bulk material (soil) and a tool (tine) was already studied and modelled in our research group with the use of zero-thickness element (Tamás et al. 2013), and the next step was to create a one-way coupled simulation.
There are commercial DEM and FEM software (e.g. EDEM and ANSYS) available that offer an interface to establish a connection, but in our study, the open source Yade (Šmilauer et al. 2015) was chosen as a DEM software to couple with ANSYS Workbench 18.2 FEM program. As this is a novel combination, a new way of connection had to be created.

DEM Model

In DEM simulations, the simplest and oldest element type is the sphere. It is widely used for modelling cohesive granular materials, like soil. However, more complex element shapes exist, for example polyhedra, which are excellent for modelling crushed rock aggregates (Orosz et al. 2017).
As there are several applications for one-way coupling, which uses spheres, the more uncommon polyhedral elements were chosen. They are randomly created based on Voronoi method (Asahina and Bolander 2011) with the desired size and shape (aspect ratio). The material of the particles is ideally rigid, and the stiffness of the real rocks is modelled with the model of the contact forces.
The constitutional model (Eliáš 2014) is cohesionless, (normal) compression and shear force is included. The normal force (F_n [N], Equation (1)) is linearly proportional with the common volume (V_c [m^3]) of the ideally rigid elements that come into contact where the factor k_n [N/m^3] is called the volumetric normal stiffness.

$$F_n = k_n V_c \qquad (1)$$

The shear force (F_s [N], Equation (2)) is linearly proportional with the relative rotations and displacements (u_s [m]) of the elements, where the factor is the shear stiffness (k_s [N/m]). The value of the shear force is maximized by the coulomb friction law (Equation (3)) where φ [-] is the inter-particle friction coefficient.

$$F_s = k_s u_s \qquad (2)$$

$$F_s \le F_n tan\varphi \qquad (3)$$

The model was tested with the modelling of a uniaxial compression test (Figure 6) in a former study (Orosz et al. 2017).

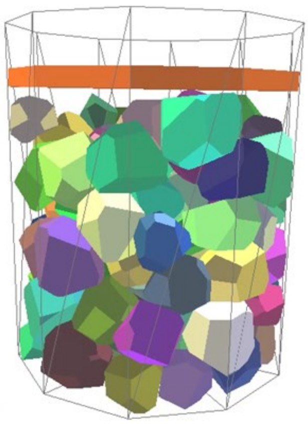

Figure 6: Uniaxial Compression Simulation of a Pack of Polyhedral Elements (Orosz et al. 2017)

Two geometrical models were created with the application of the polyhedral model using one rock: a press and a drop simulation.
In the case of the press test, a random polyhedron was created with a 100x100x100 mm bounding cube and a wall element was placed under it. Then gravity (9,81 m/s^2) was applied and the polyhedron fell onto the wall. The simulation was continued until equilibrium was reached. The wall was replaced with a plate made up from triangular facet elements. The polyhedron was compressed from upwards with another wall element (Figure 7) with a constant velocity until reaching the predetermined maximum normal force (50 kN), that was measured on the wall. At that point the force data were saved.

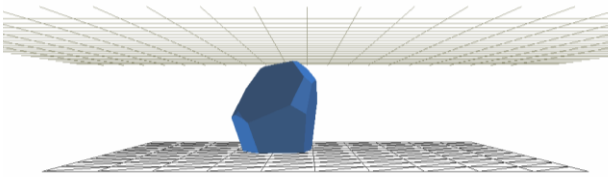

Figure 7: Compression Simulation of a Polyhedron

In the case of the drop test, the same, randomly created polyhedral element was falling onto the same plate under the influence of gravity (9,81 m/s^2) from 500 mm height and with an initial vertical velocity of 10 m/s (Figure 8). The forces were saved when the polyhedron was at its lowest position (maximum penetration into the triangular facets).

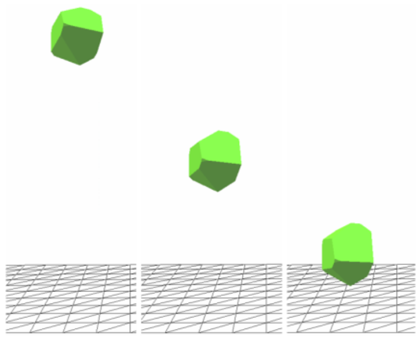

Figure 8: Free-Fall Simulation of a Polyhedron

FEM Model

The elaborated model was created in ANSYS Workbench V18.2. (ANSYS 2017). A simple prismatic body was used to model the ground which was contacted with the rock in the DEM simulation. During the FE analysis the same mesh was produced on the top surface of the body as in the DEM simulation. 10-nodes quadratic tetrahedron elements was used. A fix constrain was applied (which locked all of the 6 DoF) on the bottom surface of the solid body. Figure 9 shows the used geometry and the mesh during the FE simulation.

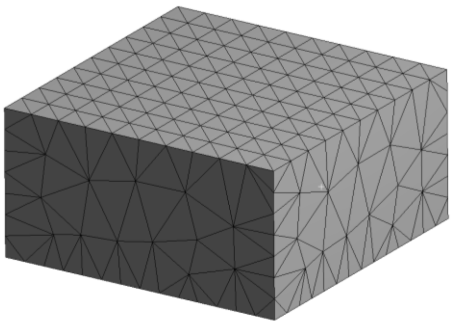

Figure 9: Geometry and the mesh used during the FE analysis

The Connection

A method was created to establish a one-way connection between Yade and ANSYS. The arising forces on the centre of mass of the triangular facets were saved in the appropriate time and were saved in a text file with a special format, containing their magnitude and coordinate of application. This file was imported into ANSYS after the creation of the proper geometry. The forces were interpolated onto the FE nodes with the so-called "mapping" technique.

RESULTS

Press Test

The interactions and magnitude of normal forces between the polyhedron-upper plate (upper, red cylinder) and the polyhedron-triangular facets are shown on Figure 10 at the time of the maximum load.

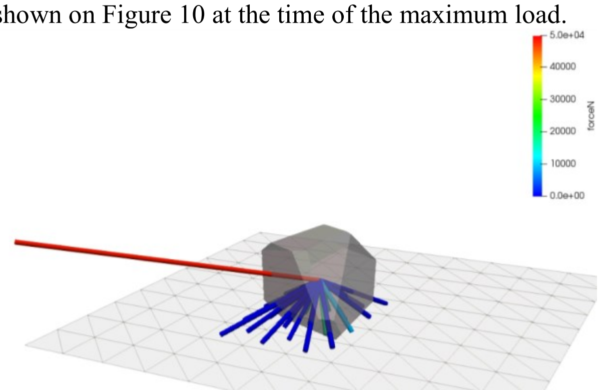

Figure 10: Normal Interactions During the Compression Simulation [N]

With the exporting of the forces acting on the triangular facets and mapping them onto the FE mesh, the Von Mises equivalent stresses and deformations can be computed (Figure 11). The effect of sharp edges and corners can be observed on the stress distribution of the prismatic body.

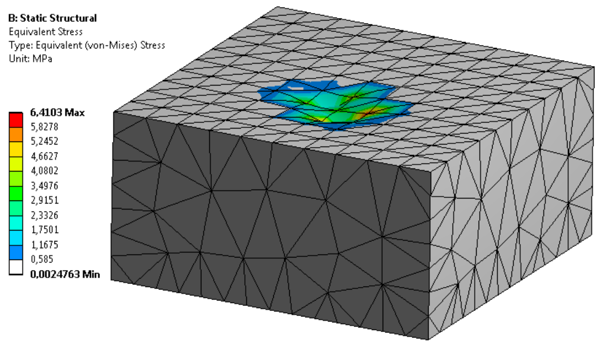

Figure 11: Von Mises Equivalent stresses [MPa] on Deformed Geometry (Deformation Scale 9100:1)

Drop Test

Figure 12 shows the interactions between the polyhedron and the triangular facets at the moment of maximum forces in case of drop test. The difference between magnitudes are easy to see, which is the result of that only one corner touches the surface of the simulated body.

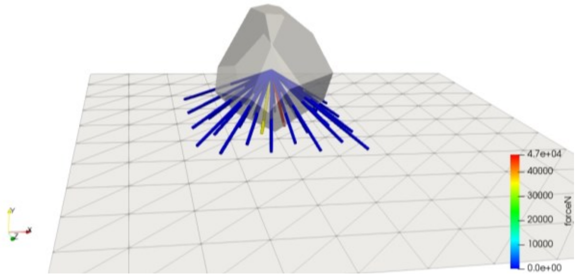

Figure 12: Normal Interactions During the Drop Simulation [N]

The effect of the sharp corner can be seen on the Von Mises stress field of the affected body (Figure 13) where the enlarged deformations also illustrate the influence of the single polyhedron.

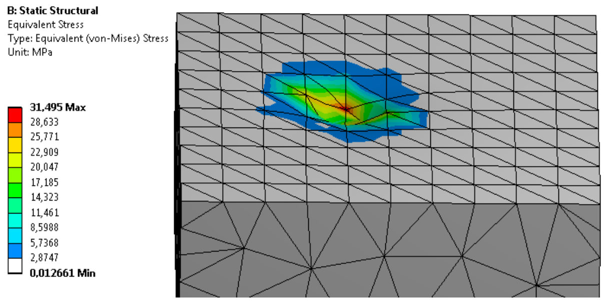

Figure 13: Von Mises Equivalent stresses [MPa] on Deformed Geometry (Deformation Scale 2000:1)

CONCLUSIONS

The introduced examples showed that there are many fields where machines interact with bulk materials and the modelling of these processes can help to improve the design and reduce cost and time.
The following conclusions were made about different techniques to model the tool of the machines:

- Zero thickness elements: fast, but only gives information about the bulk material and forces on the tool
- Cohesive constitutional: has many possibility, but hard to create
- One-way coupled simulation: gives information about stress and deformations. Fast, but only usable in small tool deformation range.
- Two-way coupling: is usable at large deformations also, but hard to define and execute due to the need of iterations.

The paper also showed that it is possible to connect a free source DEM (Yade) and a commercially available FEM software (ANSYS) in order to perform one-way coupled simulations, and a workaround was created.
The polyhedral elements are also capable for coupled simulations and can model particles that have sharp edges and corners effectively.

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AUTHOR BIOGRAPHIES

ÁKOS OROSZ is a PhD student at the Budapest University of Technology and Economics, Hungary where he received his MSc degree. His research topic is the DEM modelling of crushed stones. He is also a member of a research group in the field of discrete element modelling. His e-mail address is: orosz.akos@gt3.bme.hu and his web-page can be found at http://gt3.bme.hu/oroszakos.

KORNÉL TAMÁS is an assistant professor at Budapest University of Technology and Economics where he received his MSc degree and then completed his PhD degree. His professional field is the modelling of granular materials with the use of discrete element method (DEM). His e-mail address is: tamas.kornel@gt3.bme.hu and his web-page can be found at http://gt3.bme.hu/tamaskornel.

JÁNOS P. RÁDICS is an assistant professor at Budapest University of Technology and Economics where he received his MSc degree. He completed his PhD degree at Szent István University, Gödöllő. His main research is simulation of soil respiration after different tillage methods, and he also takes part in the DEM simulation research group of the department. His e-mail address is: radics.janos@gt3.bme.hu and his web-page can be found at http://gt3.bme.hu/radics.

PÉTER T. ZWIERCZYK is an assistant professor at Budapest University of Technology and Economics Department of Machine and Product Design where he received his M.Sc. degree and then completed his Ph.D. in mechanical engineering. His main research field is the railway wheel-rail connection. He is member of the finite element modelling (FEM) research group. His e-mail address is: z.peter@gt3.bme.hu and his web-page can be found at http://gt3.bme.hu/zwierczykpetertamas.